

PII: S0301-0104(00)00328-1

Chemical Physics 261 (2000) 491–495

Chemical Physics

www.elsevier.nl/locate/chemphys

Author index

Allwood, D.A. and P.E. Dyer, Quantitative fluorescence measurements performed on	
typical matrix molecules in matrix-assisted laser desorption/ionisation	261 (2000) 457
Alvarez, F., A. Arbe and J. Colmenero, Methyl group dynamics above the glass	
transition temperature: a molecular dynamics simulation in polyisoprene	261 (2000) 47
Arbe, A., see Alvarez, F.	261 (2000) 47
Argyrakis, P. and R. Kopelman, Random walks and reactions on dendrimer structures	261 (2000) 391
Artacho, E., see Plazanet, M.	261 (2000) 189
Bartkowiak, W. and T. Misiaszek, Solvent effect on static vibrational and electronic contribution of first-order hyperpolarizability of π -conjugated push-pull molecules:	
quantum-chemical calculations	261 (2000) 353
Bedrov, D., see Trouw, F.	261 (2000) 137
Bée, M., see Morelon, ND.	261 (2000) 75
Bellissent-Funel, MC., see Hinsen, K.	261 (2000) 25
Borodin, O., see Trouw, F.	261 (2000) 137
Boudjada, F., see Meinnel, J.	261 (2000) 165
Bouloussa, O., see Gaigeot, MP.	261 (2000) 217
Braden, D.A., see Hudson, B.S.	261 (2000) 249
Brion, C.E., see Litvinyuk, I.V.	261 (2000) 289
Bug, A.L.R. and G.J. Martyna, Calculation of neutron spectra for hydrogen in zeolites:	
rotational motions and translational motions in the Born-Oppenheimer limit	261 (2000) 89
Calaminici, P., see Reis, H.	261 (2000) 359
Cannistraro, S., see Paciaroni, A.	261 (2000) 39
Chu, SY., see Liao, HY.	261 (2000) 275
Colmenero, J., see Alvarez, F.	261 (2000) 47
Combet, J., see Morelon, ND.	261 (2000) 75
Coulombeau, C., see Gaigeot, MP.	261 (2000) 217
Cousson, A., see Meinnel, J.	261 (2000) 165
Dellerue, S., see Hinsen, K.	261 (2000) 25
Desmedt, A., see Soetens, JC.	261 (2000) 125
Drożdżyński, J., see Karbowiak, M.	261 (2000) 301
Dyer, P.E., see Allwood, D.A.	261 (2000) 457
Eckert, J., see Henson, N.J.	261 (2000) 111

Fernández-Díaz, M.T., see Plazanet, M.	261 (2000) 189
Fernández-Gómez, M., see Partal, F.	261 (2000) 239
Gaigeot, MP., N. Leulliot, M. Ghomi, H. Jobic, C. Coulombeau and O. Bouloussa,	
Analysis of the structural and vibrational properties of RNA building blocks by	
means of neutron inelastic scattering and density functional theory calculations	261 (2000) 217
Gajek, Z., see Karbowiak, M.	261 (2000) 301
Gale, J.D., see Plazanet, M.	261 (2000) 189
Gamba, Z., see Pastorino, C.	261 (2000) 317
Garcia, A., see Plazanet, M.	261 (2000) 189
Ghomi, M., see Gaigeot, MP.	261 (2000) 217
Gödicke, B., A. Langenscheidt, H. Meyer and A. Schweig, Photoinduced formation of	, , , , , , , , , , , , , , , , , , , ,
persistent contact ion pairs in solid noble gases: UV/Vis spectroscopic, photokinetic	
and energetic investigations	261 (2000) 339
Graener, H., see Patzlaff, T.	261 (2000) 381
Granucci, G., see Santoro, F.	261 (2000) 489
Guillaume, F., see Soetens, JC.	261 (2000) 125
Gulbinas, V., Transient absorption of photoexcited titanylphthalocyanine in various	
molecular arrangements	261 (2000) 469
Harris, K.D.M., see Soetens, JC.	261 (2000) 125
Hautecler, S., see Vorderwisch, P.	261 (2000) 157
Hay, P.J., see Henson, N.J.	261 (2000) 111
Henson, N.J., J. Eckert, P.J. Hay and A. Redondo, Adsorption of ethane and ethene in	264 (2000) 444
Na-Y studied by inelastic neutron scattering and computation	261 (2000) 111
Herman, H., see Parker, S.F.	261 (2000) 261
Hinsen, K., AJ. Petrescu, S. Dellerue, MC. Bellissent-Funel and G.R. Kneller,	261 (2000) 25
Harmonicity in slow protein dynamics	261 (2000) 25
Holmlid, L., see Wang, J.	261 (2000) 481
Huang, L.C.L., J.L. Lin and W.B. Tzeng, Mass analyzed threshold ionization	261 (2000) 440
spectroscopy of 4-aminobenzonitrile cation Hudson P.S. J.S. Tsa M.Z. Zeigrahi, S.E. Borker, D.A. Braden and C. Middleton The	261 (2000) 449
Hudson, B.S., J.S. Tse, M.Z. Zgierski, S.F. Parker, D.A. Braden and C. Middleton, The	
inelastic incoherent neutron spectrum of crystalline oxamide: experiment and simulation of a solid	261 (2000) 249
simulation of a solid	201 (2000) 249
Izotov, D.E. and V.P. Tarasov, Spin-lattice relaxation of deuterons at multiaxial	
reorientation of the XD ₄ tetrahedron	261 (2000) 399
Janich, M., see Patzlaff, T.	261 (2000) 381
Jobic, H., see Gaigeot, MP.	261 (2000) 217
Johnson, M., see Meinnel, J.	261 (2000) 165
Johnson, M.R., see Plazanet, M.	261 (2000) 189
Jug, K., see Reis, H.	261 (2000) 359
Varbawiak M. 7 Caiak and I Davidinashi Abanatian materials at 1	
Karbowiak, M., Z. Gajek and J. Drożdżyński, Absorption spectra analysis of hydrated	261 (2000) 201
uranium(III) complex chlorides Verrley G. L. see Verderwisch P.	261 (2000) 301
Kearley, G.J., see Vorderwisch, P. Kearley, G.J., see Plazanet, M.	261 (2000) 157 261 (2000) 189
Reality, G.J., See Flazallet, IVI.	201 (2000) 189

Kearley, G.J., see Partal, F.	261 (2000) 239
Kearley, G.J., see Johnson, M.R.	261 (2000) 555
Kneller, G.R., Inelastic neutron scattering from damped collective vibrations of	Partial P. M. Ferri
macromolecules	261 (2000) 1
Kneller, G.R., see Hinsen, K.	261 (2000) 25
Kohler, HH., see Woelki, S.	261 (2000) 411
Kohler, HH., see Woelki, S.	261 (2000) 421
Kopelman, R., see Argyrakis, P.	261 (2000) 391
Köster, A.M., see Reis, H.	261 (2000) 359
Kubanek, F., see Vorderwisch, P.	261 (2000) 157
Langenscheidt, A., see Gödicke, B.	261 (2000) 339
Leulliot, N., see Gaigeot, MP.	261 (2000) 217
Liao, HY., MD. Su and SY. Chu, Density functional studies on the mechanisms of	` /
unimolecular reactions of HXCSe $(X = H, F, Cl, and Br)$	261 (2000) 275
Lin, J.L., see Huang, L.C.L.	261 (2000) 449
Litvinyuk, I.V., Y. Zheng and C.E. Brion, Electron momentum spectroscopy study of	,
amantadine: binding energy spectra and valence orbital electron density distributions	
López-González, J.J., see Partal, F.	261 (2000) 239
TO DO SALIDE	201 (2000) 237
Malézieux, B., see Raupach, E.	261 (2000) 373
Mani, M., see Meinnel, J.	261 (2000) 165
Martyna, G.J., see Bug, A.L.R.	261 (2000) 89
Maus, M. and W. Rettig, The influence of conformation and energy gaps on optical	
transition moments in donor-acceptor biphenyls	261 (2000) 323
McGreevy, R.L., see Mellergård, A.	261 (2000) 267
Meinnel, J., M. Mani, A. Cousson, F. Boudjada, W. Paulus and M. Johnson, Structure	
of trihalogenomesitylenes and tunneling of the methyl groups protons	261 (2000) 165
Mellergård, A. and R.L. McGreevy, Recent developments of the RMCPOW method for	
structural modelling	261 (2000) 267
Meyer, H., see Gödicke, B.	261 (2000) 339
Middleton, C., see Hudson, B.S.	261 (2000) 249
Misiaszek, T., see Bartkowiak, W.	261 (2000) 353
Mitra, S., R. Mukhopadhyay and K. Venu, Molecular motions in liquid crystal BBBA	
(4O.4): QENS study	261 (2000) 149
Monkenbusch, M., see Smith, G.D.	261 (2000) 61
Morelon, ND., M. Bée and J. Combet, Molecular dynamics simulation of a channel	Sicrytula, P.O., ved
type inclusion compound: comparison with neutron scattering experiments	261 (2000) 75
Mukhopadhyay, R., see Mitra, S.	261 (2000) 149
Navarro, A., see Partal, F.	261 (2000) 239
Ordejón, P., see Plazanet, M.	261 (2000) 189
Paciaroni, A., F. Sacchetti and S. Cannistraro, A Monte Carlo analysis of the elastic	
incoherent neutron scattering data in hydrated azurin	201 (2000) 39
incoherent neutron scattering data in hydrated azurin Papadopoulos, M.G., see Reis, H.	261 (2000) 39 261 (2000) 359

Parker, S.F., H. Herman, A. Zimmerman and K.P.J. Williams, The vibrational	
spectrum of K ₂ PdCl ₄ : first detection of the silent mode v ₅	261 (2000) 261
Partal, F., M. Fernández-Gómez, J.J. López-González, A. Navarro and G.J. Kearley,	201 (2000) 201
Vibrational analysis of the inelastic neutron scattering spectrum of pyridine	261 (2000) 239
Pastorino, C. and Z. Gamba, Study of sulfur α -S ₈ crystals with an anisotropic inter-	201 (2000) 257
molecular potential model	261 (2000) 317
Patzlaff, T., M. Janich, G. Seifert and H. Graener, Ultrafast dynamics of water-AOT-	201 (2000) 317
octane microemulsions	261 (2000) 381
Paul, W., see Smith, G.D.	261 (2000) 61
Paulus, W., see Meinnel, J.	261 (2000) 165
Persico, M., see Santoro, F.	261 (2000) 489
Petrescu, AJ., see Hinsen, K.	261 (2000) 489
Petrongolo, C., see Santoro, F.	261 (2000) 489
Plazanet, M., M.R. Johnson, J.D. Gale, T. Yildirim, G.J. Kearley, M.T. Fernández-	201 (2000) 409
Díaz, D. Sánchez-Portal, E. Artacho, J.M. Soler, P. Ordejón, A. Garcia and H.P.	
Trommsdorff, The structure and dynamics of crystalline durene by neutron	261 (2000) 100
scattering and numerical modelling using density functional methods	261 (2000) 189
Raupach, E., G.L.J.A. Rikken, C. Train and B. Malézieux, Modelling of magneto-	
chiral enantioselective photochemistry	261 (2000) 373
Redondo, A., see Henson, N.J.	261 (2000) 111
Reis, H., M.G. Papadopoulos, P. Calaminici, K. Jug and A.M. Köster, Calculation of	201 (2000) 111
macroscopic linear and nonlinear optical susceptibilities for the naphthalene,	
anthracene and <i>meta</i> -nitroaniline crystals	261 (2000) 359
Rettig, W., see Maus, M.	261 (2000) 323
Richter, D., see Smith, G.D.	261 (2000) 61
Rikken, G.L.J.A., see Raupach, E.	261 (2000) 373
Rikkeli, G.L.J.A., see Raupaeli, E.	201 (2000) 373
Sacchetti, F., see Paciaroni, A.	261 (2000) 39
Sánchez-Portal, D., see Plazanet, M.	261 (2000) 189
Santoro, F., C. Petrongolo, G. Granucci and M. Persico, Erratum to "Quantum and	
semiclassical dynamics of the Franck-Condon wave packet on the coupled potential	
surfaces of the NO ₂ $\tilde{X}^2A'/\tilde{A}^2A'$ conical intersection" [Chemical Physics 259 (2000)	
193–200]	261 (2000) 489
Schweig, A., see Gödicke, B.	261 (2000) 339
Seifert, G., see Patzlaff, T.	261 (2000) 381
Skrylnik, P.G., see Ziatdinov, A.M.	261 (2000) 439
Smith, G.D., W. Paul, M. Monkenbusch and D. Richter, A comparison of neutron	
scattering studies and computer simulations of polymer melts	261 (2000) 61
Smith, G.D., see Trouw, F.	261 (2000) 137
Soetens, JC., A. Desmedt, F. Guillaume and K.D.M. Harris, Molecular dynamics	
simulation study of cyclohexane guest molecules in the cyclohexane/thiourea	
inclusion compound	261 (2000) 125
Soler, J.M., see Plazanet, M.	261 (2000) 189
Su, MD., see Liao, HY.	261 (2000) 275
WE WORLD TO THE THE WAY TO SEE THE W	2000) 210
Tarasov, V.P., see Izotov, D.E.	261 (2000) 399
Train, C., see Raupach, E.	261 (2000) 373

Trommsdorff, H.P., see Plazanet, M.	261 (2000) 189
Trouw, F., D. Bedrov, O. Borodin and G.D. Smith, Diffusion in aqueous solutions of	(,,
1,2-dimethoxyethane: comparison of molecular dynamics simulations and quasi-	
elastic neutron scattering	261 (2000) 137
Tse, J.S., see Hudson, B.S.	261 (2000) 249
Tzeng, W.B., see Huang, L.C.L.	261 (2000) 449
Venu, K., see Mitra, S.	261 (2000) 149
Vorderwisch, P., S. Hautecler, G.J. Kearley and F. Kubanek, Influence of the guest	
molecule on the rotational potential for NH3 groups in Hofmann clathrates	261 (2000) 157
Wang, J. and L. Holmlid, Formation of long-lived Rydberg states of H ₂ at K	
impregnated surfaces	261 (2000) 481
Williams, K.P.J., see Parker, S.F.	261 (2000) 261
Woelki, S. and HH. Kohler, A modified Poisson-Boltzmann equation. I. Basic	
relations	261 (2000) 411
Woelki, S. and HH. Kohler, A modified Poisson-Boltzmann equation. II. Models and	
solutions	261 (2000) 421
Yildirim, T., see Plazanet, M.	261 (2000) 189
Yildirim, T., Structure and dynamics from combined neutron scattering and first-	
principles studies	261 (2000) 205
Zgierski, M.Z., see Hudson, B.S.	261 (2000) 249
Zheng, Y., see Litvinyuk, I.V.	261 (2000) 289
Ziatdinov, A.M. and P.G. Skrylnik, Graphite intercalation by nitric acid: conduction	,
ESR and theoretical studies	261 (2000) 439
Zimmerman, A., see Parker, S.F.	261 (2000) 261



Chemical Physics 261 (2000) 497-508

Chemical Physics

www.elsevier.nl/locate/chemphys

Subject index

Methods and constructs

Theoretical

261 (2000) 205
261 (2000) 220
261 (2000) 239
261 (2000) 275
261 (2000) 289
261 (2000) 301
American de la companya de la compan
261 (2000) 189
201 (2000) 189
261 (2000) 217
261 (2000) 217
261 (2000) 249
261 (2000) 301

PII: S0301-0104(00)00329-3

biojett mater venemaa i nysies 201 (2000) 157 500	
Study of sulfur α -S ₈ crystals with an anisotropic inter-molecular potential model, C.	261 (2000) 217
Pastorino and Z. Gamba The influence of conformation and energy gaps on optical transition moments in	261 (2000) 317
donor-acceptor biphenyls, M. Maus and W. Rettig Photoinduced formation of persistent contact ion pairs in solid noble gases: UV/Vis	261 (2000) 323
spectroscopic, photokinetic and energetic investigations, B. Gödicke, A. Langenscheidt, H. Meyer and A. Schweig	261 (2000) 339
Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)	
Solvent effect on static vibrational and electronic contribution of first-order hyperpolarizability of π -conjugated push-pull molecules: quantum-chemical calcula-	261 (2000) 252
tions, W. Bartkowiak and T. Misiaszek Calculation of macroscopic linear and nonlinear optical susceptibilities for the	261 (2000) 353
naphthalene, anthracene and <i>meta</i> -nitroaniline crystals, H. Reis, M.G. Papadopoulos, P. Calaminici, K. Jug and A.M. Köster	261 (2000) 359
Reactive molecular dynamics including dissipative processes	
Modelling of magneto-chiral enantioselective photochemistry, E. Raupach, G.L.J.A. Rikken, C. Train and B. Malézieux	261 (2000) 373
Intramolecular dynamics	
Study of sulfur α-S ₈ crystals with an anisotropic inter-molecular potential model, C. Pastorino and Z. Gamba	261 (2000) 317
mid 1/4.8 time its 1/	201 (2000) 317
Molecular dynamics of many particle systems and condensed phases	
Harmonicity in slow protein dynamics, K. Hinsen, AJ. Petrescu, S. Dellerue, MC. Bellissent-Funel and G.R. Kneller	261 (2000) 25
Methyl group dynamics above the glass transition temperature: a molecular dynamics simulation in polyisoprene, F. Alvarez, A. Arbe and J. Colmenero	261 (2000) 47
A comparison of neutron scattering studies and computer simulations of polymer melts, G.D. Smith, W. Paul, M. Monkenbusch and D. Richter	261 (2000) 61
Molecular dynamics simulation of a channel type inclusion compound: comparison	, ,
with neutron scattering experiments, ND. Morelon, M. Bée and J. Combet Molecular dynamics simulation study of cyclohexane guest molecules in the	261 (2000) 75
cyclohexane/thiourea inclusion compound, JC. Soetens, A. Desmedt, F. Guillaume	
and K.D.M. Harris Study of sulfur α -S ₈ crystals with an anisotropic inter-molecular potential model, C.	261 (2000) 125
Pastorino and Z. Gamba	261 (2000) 317
Ultrafast dynamics of water-AOT-octane microemulsions, T. Patzlaff, M. Janich, G.	
Seifert and H. Graener	261 (2000) 381
Statistical computational methods (incl. Monte Carlo)	
Adsorption of ethane and ethene in Na-Y studied by inelastic neutron scattering and	ton mbath.
computation, N.J. Henson, J. Eckert, P.J. Hay and A. Redondo Recent developments of the RMCPOW method for structural modelling, A. Mellergård	261 (2000) 111
and R.L. McGreevy	261 (2000) 267
Random walks and reactions on dendrimer structures, P. Argyrakis and R. Kopelman	261 (2000) 391

 Inelastic neutron scattering from damped collective vibrations of macromolecules, G.R. Kneller Harmonicity in slow protein dynamics, K. Hinsen, AJ. Petrescu, S. Dellerue, MC. Bellissent-Funel and G.R. Kneller A comparison of neutron scattering studies and computer simulations of polymer melts, G.D. Smith, W. Paul, M. Monkenbusch and D. Richter Spin-lattice relaxation of deuterons at multiaxial reorientation of the XD4 tetrahedron, D.E. Izotov and V.P. Tarasov Fluctuations and random processes Inelastic neutron scattering from damped collective vibrations of macromolecules, G.R. Kneller 	261 (2000) 61
Bellissent-Funel and G.R. Kneller A comparison of neutron scattering studies and computer simulations of polymer melts, G.D. Smith, W. Paul, M. Monkenbusch and D. Richter Spin-lattice relaxation of deuterons at multiaxial reorientation of the XD ₄ tetrahedron, D.E. Izotov and V.P. Tarasov Fluctuations and random processes Inelastic neutron scattering from damped collective vibrations of macromolecules, G.R.	261 (2000) 25 261 (2000) 61 261 (2000) 399
G.D. Smith, W. Paul, M. Monkenbusch and D. Richter Spin-lattice relaxation of deuterons at multiaxial reorientation of the XD ₄ tetrahedron, D.E. Izotov and V.P. Tarasov Fluctuations and random processes Inelastic neutron scattering from damped collective vibrations of macromolecules, G.R.	nomini di
D.E. Izotov and V.P. Tarasov Fluctuations and random processes Inelastic neutron scattering from damped collective vibrations of macromolecules, G.R.	261 (2000) 399
Inelastic neutron scattering from damped collective vibrations of macromolecules, G.R.	261 (2000) 1
	261 (2000) 1
	201 (2000)
Equilibrium statistical mechanics and thermodynamics	
A modified Poisson-Boltzmann equation. I. Basic relations, S. Woelki and HH. Kohler	261 (2000) 411
A modified Poisson-Boltzmann equation. II. Models and solutions, S. Woelki and	
HH. Kohler	261 (2000) 421
Extremum methods for ensembles (energy, entropy, free energy)	Manyana and a
A modified Poisson-Boltzmann equation. I. Basic relations, S. Woelki and HH. Kohler	261 (2000) 411
A modified Poisson-Boltzmann equation. II. Models and solutions, S. Woelki and	
HH. Kohler	261 (2000) 421
Time and space correlation functions	
Inelastic neutron scattering from damped collective vibrations of macromolecules, G.R. Kneller	261 (2000) 1
Harmonicity in slow protein dynamics, K. Hinsen, AJ. Petrescu, S. Dellerue, MC. Bellissent-Funel and G.R. Kneller	261 (2000) 25
Calculation of neutron spectra for hydrogen in zeolites: rotational motions and	Collegious succession
translational motions in the Born-Oppenheimer limit, A.L.R. Bug and G.J. Martyna Molecular dynamics simulation study of cyclohexane guest molecules in the cyclohexane/thiourea inclusion compound, JC. Soetens, A. Desmedt, F. Guillaume	261 (2000) 89
and K.D.M. Harris	261 (2000) 125
Experiment	
Magnetic resonances	
Graphite intercalation by nitric acid: conduction ESR and theoretical studies, A.M. Ziatdinov and P.G. Skrylnik	261 (2000) 439
Molecular spectroscopy	
Molecular motions in liquid crystal BBBA (40.4): QENS study, S. Mitra, R. Mukhopadhyay and K. Venu	261 (2000) 149
Analysis of the structural and vibrational properties of RNA building blocks by means of neutron inelastic scattering and density functional theory calculations, MP.	
Gaigeot, N. Leulliot, M. Ghomi, H. Jobic, C. Coulombeau and O. Bouloussa	261 (2000) 217

Absorption spectra analysis of hydrated uranium(III) complex chlorides, M. Karbow-	261 (2000) 201
iak, Z. Gajek and J. Drożdżyński Mass analyzed threshold ionization spectroscopy of 4-aminobenzonitrile cation, L.C.L.	261 (2000) 301
Huang, J.L. Lin and W.B. Tzeng	261 (2000) 449
Quantitative fluorescence measurements performed on typical matrix molecules in	
matrix-assisted laser desorption/ionisation, D.A. Allwood and P.E. Dyer	261 (2000) 457
-Raman	
The vibrational spectrum of K_2PdCl_4 : first detection of the silent mode v_5 , S.F. Parker,	
H. Herman, A. Zimmerman and K.P.J. Williams	261 (2000) 261
-UV	
Photoinduced formation of persistent contact ion pairs in solid noble gases: UV/Vis	
spectroscopic, photokinetic and energetic investigations, B. Gödicke, A. Lan-	2(1 (2000) 220
genscheidt, H. Meyer and A. Schweig	261 (2000) 339
-visible	
Modelling of magneto-chiral enantioselective photochemistry, E. Raupach, G.L.J.A.	261 (2000) 272
Rikken, C. Train and B. Malézieux	261 (2000) 373
Multiphoton ionization	
Mass analyzed threshold ionization spectroscopy of 4-aminobenzonitrile cation, L.C.L. Huang, J.L. Lin and W.B. Tzeng	261 (2000) 440
Huang, J.L. Lin and W.B. 12eng	261 (2000) 449
Electron impact spectroscopy	
Electron momentum spectroscopy study of amantadine: binding energy spectra and valence orbital electron density distributions, I.V. Litvinyuk, Y. Zheng and C.E.	
Brion	261 (2000) 289
I are induced fluorescence	and the second second
Laser induced fluorescence Quantitative fluorescence measurements performed on typical matrix molecules in	
matrix-assisted laser desorption/ionisation, D.A. Allwood and P.E. Dyer	261 (2000) 457
Ultrafast measurements	
Ultrafast dynamics of water-AOT-octane microemulsions, T. Patzlaff, M. Janich, G.	
Seifert and H. Graener	261 (2000) 381
Transient absorption of photoexcited titanylphthalocyanine in various molecular	
arrangements, V. Gulbinas	261 (2000) 469
Atomic and molecular beam techniques	
Formation of long-lived Rydberg states of H ₂ at K impregnated surfaces, J. Wang and	
L. Holmlid	261 (2000) 481
X-ray, electron and neutron diffraction	
Recent developments of the RMCPOW method for structural modelling, A. Mellergård	261 (2000) 262
and R.L. McGreevy	261 (2000) 267
Neutron scattering (inelastic and quasielastic)	
A Monte Carlo analysis of the elastic incoherent neutron scattering data in hydrated	261 (2000) 26
azurin, A. Paciaroni, F. Sacchetti and S. Cannistraro Methyl group dynamics above the glass transition temperature: a molecular dynamics	261 (2000) 39
simulation in polyisoprene, F. Alvarez, A. Arbe and J. Colmenero	261 (2000) 47
	(====)

A comparison of neutron scattering studies and computer simulations of polymer melts,	264 (2000) 64
G.D. Smith, W. Paul, M. Monkenbusch and D. Richter	261 (2000) 61
Molecular dynamics simulation of a channel type inclusion compound: comparison with neutron scattering experiments, ND. Morelon, M. Bée and J. Combet	261 (2000) 75
Adsorption of ethane and ethene in Na-Y studied by inelastic neutron scattering and	261 (2000) 75
computation, N.J. Henson, J. Eckert, P.J. Hay and A. Redondo	261 (2000) 111
Molecular dynamics simulation study of cyclohexane guest molecules in the cyclohexane/thiourea inclusion compound, JC. Soetens, A. Desmedt, F. Guillaume and K.D.M. Harris	
Diffusion in aqueous solutions of 1,2-dimethoxyethane: comparison of molecular dynamics simulations and quasielastic neutron scattering, F. Trouw, D. Bedrov, O.	261 (2000) 125
Borodin and G.D. Smith	261 (2000) 137
Molecular motions in liquid crystal BBBA (40.4): QENS study, S. Mitra, R.	
Mukhopadhyay and K. Venu	261 (2000) 149
Influence of the guest molecule on the rotational potential for NH ₃ groups in Hofmann	
clathrates, P. Vorderwisch, S. Hautecler, G.J. Kearley and F. Kubanek	261 (2000) 157
Structure of trihalogenomesitylenes and tunneling of the methyl groups protons, J.	
Meinnel, M. Mani, A. Cousson, F. Boudjada, W. Paulus and M. Johnson	261 (2000) 165
The structure and dynamics of crystalline durene by neutron scattering and numerical modelling using density functional methods, M. Plazanet, M.R. Johnson, J.D. Gale,	Dolf I.H has a willow to visually
T. Yildirim, G.J. Kearley, M.T. Fernández-Díaz, D. Sánchez-Portal, E. Artacho,	A 64 (AAAA) 400
J.M. Soler, P. Ordejón, A. Garcia and H.P. Trommsdorff	261 (2000) 189
Structure and dynamics from combined neutron scattering and first-principles studies, T. Yildirim	261 (2000) 205
Analysis of the structural and vibrational properties of RNA building blocks by means	261 (2000) 205
of neutron inelastic scattering and density functional theory calculations, MP.	
Gaigeot, N. Leulliot, M. Ghomi, H. Jobic, C. Coulombeau and O. Bouloussa	261 (2000) 217
Vibrational analysis of the inelastic neutron scattering spectrum of pyridine, F. Partal,	201 (2000) 217
M. Fernández-Gómez, J.J. López-González, A. Navarro and G.J. Kearley	261 (2000) 239
The inelastic incoherent neutron spectrum of crystalline oxamide: experiment and simulation of a solid, B.S. Hudson, J.S. Tse, M.Z. Zgierski, S.F. Parker, D.A.	201 (2000) 207
Braden and C. Middleton	261 (2000) 249
The vibrational spectrum of K_2PdCl_4 : first detection of the silent mode v_5 , S.F. Parker,	Absorption appoin
H. Herman, A. Zimmerman and K.P.J. Williams	261 (2000) 261
Small angle X-ray and neutron diffraction	
Structure of trihalogenomesitylenes and tunneling of the methyl groups protons, J.	
Meinnel, M. Mani, A. Cousson, F. Boudjada, W. Paulus and M. Johnson	261 (2000) 165

Objects

Bulk systems

Liquid mixtures and solutions

Diffusion in aqueous solutions of 1,2-dimethoxyethane: comparison of molecular dynamics simulations and quasielastic neutron scattering, F. Trouw, D. Bedrov, O. Borodin and G.D. Smith

261 (2000) 137

The influence of conformation and energy gaps on optical transition moments in	
donor-acceptor biphenyls, M. Maus and W. Rettig Ultrafast dynamics of water-AOT-octane microemulsions, T. Patzlaff, M. Janich, G.	261 (2000) 323
Seifert and H. Graener Transient absorption of photoexcited titanylphthalocyanine in various molecular	261 (2000) 381
arrangements, V. Gulbinas	261 (2000) 469
Crystals	
Adsorption of ethane and ethene in Na-Y studied by inelastic neutron scattering and	
computation, N.J. Henson, J. Eckert, P.J. Hay and A. Redondo	261 (2000) 111
Influence of the guest molecule on the rotational potential for NH ₃ groups in Hofmann	
clathrates, P. Vorderwisch, S. Hautecler, G.J. Kearley and F. Kubanek	261 (2000) 157
Structure and dynamics from combined neutron scattering and first-principles studies,	Inflam militaloli
T. Yildirim	261 (2000) 205
The inelastic incoherent neutron spectrum of crystalline oxamide: experiment and	
simulation of a solid, B.S. Hudson, J.S. Tse, M.Z. Zgierski, S.F. Parker, D.A. Braden and C. Middleton	261 (2000) 249
Recent developments of the RMCPOW method for structural modelling, A. Mellergård	201 (2000) 249
and R.L. McGreevy	261 (2000) 267
Study of sulfur α -S ₈ crystals with an anisotropic inter-molecular potential model, C.	
Pastorino and Z. Gamba	261 (2000) 317
Calculation of macroscopic linear and nonlinear optical susceptibilities for the	
naphthalene, anthracene and meta-nitroaniline crystals, H. Reis, M.G. Papadopou-	Structure and dyn
los, P. Calaminici, K. Jug and A.M. Köster	261 (2000) 359
-neat	
The structure and dynamics of crystalline durene by neutron scattering and numerical	
modelling using density functional methods, M. Plazanet, M.R. Johnson, J.D. Gale,	
T. Yildirim, G.J. Kearley, M.T. Fernández-Díaz, D. Sánchez-Portal, E. Artacho,	
J.M. Soler, P. Ordejón, A. Garcia and H.P. Trommsdorff	261 (2000) 189
The vibrational spectrum of K_2PdCl_4 : first detection of the silent mode v_5 , S.F. Parker,	
H. Herman, A. Zimmerman and K.P.J. Williams	261 (2000) 261
Absorption spectra analysis of hydrated uranium(III) complex chlorides, M. Karbow-	
iak, Z. Gajek and J. Drożdżyński	261 (2000) 301
Transient absorption of photoexcited titanylphthalocyanine in various molecular arrangements, V. Gulbinas	261 (2000) 460
arrangements, v. Guioinas	261 (2000) 469
Complex fluids	
-liquid crystals	
Molecular motions in liquid crystal BBBA (40.4): QENS study, S. Mitra, R.	
Mukhopadhyay and K. Venu	261 (2000) 149
Polymers	
Methyl group dynamics above the glass transition temperature: a molecular dynamics	
simulation in polyisoprene, F. Alvarez, A. Arbe and J. Colmenero	261 (2000) 47
A comparison of neutron scattering studies and computer simulations of polymer melts,	
G.D. Smith, W. Paul, M. Monkenbusch and D. Richter	261 (2000) 61

Surfaces	
A modified Poisson-Boltzmann equation. I. Basic relations, S. Woelki and HH.	
Kohler	261 (2000) 411
A modified Poisson-Boltzmann equation. II. Models and solutions, S. Woelki and	
HH. Kohler	261 (2000) 421
Low-dimensional materials	
Molecular dynamics simulation study of cyclohexane guest molecules in the cyclohexane/thiourea inclusion compound, JC. Soetens, A. Desmedt, F. Guillaume	2(1 (2000) 125
and K.D.M. Harris Pendem welks and reactions on dendrimer structures. P. Argurekis and P. Konelman	261 (2000) 125
Random walks and reactions on dendrimer structures, P. Argyrakis and R. Kopelman Graphite intercalation by nitric acid: conduction ESR and theoretical studies, A.M.	261 (2000) 391
Ziatdinov and P.G. Skrylnik	261 (2000) 439
Microscopic and mesoscopic systems	
Molecules (neutral and ionic)	
Diffusion in aqueous solutions of 1,2-dimethoxyethane: comparison of molecular dynamics simulations and quasielastic neutron scattering, F. Trouw, D. Bedrov, O.	hdmlott _1 201 (200) 450
Borodin and G.D. Smith	261 (2000) 137
Density functional studies on the mechanisms of unimolecular reactions of HXCSe (X = H, F, Cl, and Br), HY. Liao, MD. Su and SY. Chu	261 (2000) 275
Solvent effect on static vibrational and electronic contribution of first-order	
hyperpolarizability of π -conjugated push–pull molecules: quantum-chemical calculations, W. Bartkowiak and T. Misiaszek	261 (2000) 252
Modelling of magneto-chiral enantioselective photochemistry, E. Raupach, G.L.J.A.	261 (2000) 353
Rikken, C. Train and B. Malézieux	261 (2000) 373
Spin-lattice relaxation of deuterons at multiaxial reorientation of the XD ₄ tetrahedron,	
D.E. Izotov and V.P. Tarasov	261 (2000) 399
Mass analyzed threshold ionization spectroscopy of 4-aminobenzonitrile cation, L.C.L.	smulf@magdlfell
Huang, J.L. Lin and W.B. Tzeng	261 (2000) 449
Quantitative fluorescence measurements performed on typical matrix molecules in matrix-assisted laser desorption/ionisation, D.A. Allwood and P.E. Dyer	261 (2000) 457
Formation of long-lived Rydberg states of H ₂ at K impregnated surfaces, J. Wang and	201 (2000) 437
L. Holmlid	261 (2000) 481
-diatomic	
Calculation of neutron spectra for hydrogen in zeolites: rotational motions and translational motions in the Born-Oppenheimer limit, A.L.R. Bug and G.J. Martyna	261 (2000) 89
small polyatomics	
-small polyatomics Vibrational analysis of the inelastic neutron scattering spectrum of pyridine, F. Partal,	
M. Fernández-Gómez, J.J. López-González, A. Navarro and G.J. Kearley	261 (2000) 239
-polymeric and biological	
Inelastic neutron scattering from damped collective vibrations of macromolecules, G.R.	
Kneller	261 (2000) 1

Electron momentum anothercomy study of amountading hinding anony spectra and	
Electron momentum spectroscopy study of amantadine: binding energy spectra and valence orbital electron density distributions, I.V. Litvinyuk, Y. Zheng and C.E.	
Brion	261 (2000) 289
-Betroom equator 11 Models and volument. S. Weellin and a trained	
Molecular aggregates	
Molecular dynamics simulation of a channel type inclusion compound: comparison	
with neutron scattering experiments, ND. Morelon, M. Bée and J. Combet	261 (2000) 75
Photoinduced formation of persistent contact ion pairs in solid noble gases: UV/Vis spectroscopic, photokinetic and energetic investigations, B. Gödicke, A. Lan-	
genscheidt, H. Meyer and A. Schweig	261 (2000) 339
	201 (2000) 333
-van der Waals molecules	
Structure and dynamics from combined neutron scattering and first-principles studies,	
T. Yildirim	261 (2000) 205
-clusters	
Formation of long-lived Rydberg states of H ₂ at K impregnated surfaces, J. Wang and	261 (2000) 401
L. Holmlid	261 (2000) 481
-complexes	
Absorption spectra analysis of hydrated uranium(III) complex chlorides, M. Karbow-	Dennity, Junebonn
iak, Z. Gajek and J. Drożdżyński	261 (2000) 301
Supramolecular assemblies (incl. nanoparticles and nanostructures)	
Ultrafast dynamics of water-AOT-octane microemulsions, T. Patzlaff, M. Janich, G.	
Seifert and H. Graener	261 (2000) 381
Proteins	
Harmonicity in slow protein dynamics, K. Hinsen, AJ. Petrescu, S. Dellerue, MC.	
Bellissent-Funel and G.R. Kneller	261 (2000) 25
A Monte Carlo analysis of the elastic incoherent neutron scattering data in hydrated	
azurin, A. Paciaroni, F. Sacchetti and S. Cannistraro	261 (2000) 39
Nucleic acids	
Analysis of the structural and vibrational properties of RNA building blocks by means	
of neutron inelastic scattering and density functional theory calculations, MP.	
Gaigeot, N. Leulliot, M. Ghomi, H. Jobic, C. Coulombeau and O. Bouloussa	261 (2000) 217
nume in the Burns-Oppenheures family A.2.2. Burg and C.J. Marryra. 241,120001, NV	
Phenomena	
Molecular structure	
Structure of trihalogenomesitylenes and tunneling of the methyl groups protons, J.	
Meinnel, M. Mani, A. Cousson, F. Boudjada, W. Paulus and M. Johnson	261 (2000) 165
The influence of conformation and energy gaps on optical transition moments in	norther purchal
donor-acceptor biphenyls, M. Maus and W. Rettig	261 (2000) 323

Mass analyzed threshold ionization spectroscopy of 4-aminobenzonitrile cation, L.C.L.	244 (224)
Huang, J.L. Lin and W.B. Tzeng	261 (2000) 449
Vibrations and rotations of molecules	
Calculation of neutron spectra for hydrogen in zeolites: rotational motions and	
translational motions in the Born-Oppenheimer limit, A.L.R. Bug and G.J. Martyna Influence of the guest molecule on the rotational potential for NH ₃ groups in Hofmann	261 (2000) 89
clathrates, P. Vorderwisch, S. Hautecler, G.J. Kearley and F. Kubanek	261 (2000) 157
The structure and dynamics of crystalline durene by neutron scattering and numerical modelling using density functional methods, M. Plazanet, M.R. Johnson, J.D. Gale, T. Yildirim, G.J. Kearley, M.T. Fernández-Díaz, D. Sánchez-Portal, E. Artacho,	
J.M. Soler, P. Ordejón, A. Garcia and H.P. Trommsdorff	261 (2000) 189
Structure and dynamics from combined neutron scattering and first-principles studies,	201 (2000) 102
T. Yildirim	261 (2000) 205
Analysis of the structural and vibrational properties of RNA building blocks by means	201 (2000) 200
of neutron inelastic scattering and density functional theory calculations, MP.	
Gaigeot, N. Leulliot, M. Ghomi, H. Jobic, C. Coulombeau and O. Bouloussa Vibrational analysis of the inelastic neutron scattering spectrum of pyridine, F. Partal,	261 (2000) 217
M. Fernández-Gómez, J.J. López-González, A. Navarro and G.J. Kearley	261 (2000) 239
The vibrational spectrum of K ₂ PdCl ₄ : first detection of the silent mode v ₅ , S.F. Parker,	muldheddid
H. Herman, A. Zimmerman and K.P.J. Williams	261 (2000) 261
Electronic structure and states	
Electron momentum spectroscopy study of amantadine: binding energy spectra and valence orbital electron density distributions, I.V. Litvinyuk, Y. Zheng and C.E.	
Brion	261 (2000) 289
Molecular interactions	
Adsorption of ethane and ethene in Na-Y studied by inelastic neutron scattering and	
computation, N.J. Henson, J. Eckert, P.J. Hay and A. Redondo	261 (2000) 111
Structure of trihalogenomesitylenes and tunneling of the methyl groups protons, J.	, ,
Meinnel, M. Mani, A. Cousson, F. Boudjada, W. Paulus and M. Johnson	261 (2000) 165
Study of sulfur α -S ₈ crystals with an anisotropic inter-molecular potential model, C.	
Pastorino and Z. Gamba	261 (2000) 317
Transient absorption of photoexcited titanylphthalocyanine in various molecular	
arrangements, V. Gulbinas	261 (2000) 469
Spectral bandshapes and intensities	
Calculation of neutron spectra for hydrogen in zeolites: rotational motions and	
translational motions in the Born-Oppenheimer limit, A.L.R. Bug and G.J. Martyna	261 (2000) 89
Energy transfer processes	
Ultrafast dynamics of water-AOT-octane microemulsions, T. Patzlaff, M. Janich, G.	
Seifert and H. Graener	261 (2000) 381
Transient absorption of photoexcited titanylphthalocyanine in various molecular	
arrangements, V. Gulbinas	261 (2000) 469

Molecular photophysical processes	
Photoinduced formation of persistent contact ion pairs in solid noble gases: UV/Vis	
spectroscopic, photokinetic and energetic investigations, B. Gödicke, A. Lan-	2(1 (2000) 220
genscheidt, H. Meyer and A. Schweig	261 (2000) 339
Quantitative fluorescence measurements performed on typical matrix molecules in	261 (2000) 457
matrix-assisted laser desorption/ionisation, D.A. Allwood and P.E. Dyer	261 (2000) 457
Photochemistry	
Modelling of magneto-chiral enantioselective photochemistry, E. Raupach, G.L.J.A.	
Rikken, C. Train and B. Malézieux	261 (2000) 373
AND THE PROPERTY OF THE PROPER	
Intramolecular dynamics	
Inelastic neutron scattering from damped collective vibrations of macromolecules, G.R.	
Kneller	261 (2000) 1
Spin-lattice relaxation of deuterons at multiaxial reorientation of the XD ₄ tetrahedron,	Apalysis of the str
D.E. Izotov and V.P. Tarasov	261 (2000) 399
CVP protein white or the company of	
-protein motion	
Harmonicity in slow protein dynamics, K. Hinsen, AJ. Petrescu, S. Dellerue, MC.	
Bellissent-Funel and G.R. Kneller	261 (2000) 25
A Monte Carlo analysis of the elastic incoherent neutron scattering data in hydrated	A management of
azurin, A. Paciaroni, F. Sacchetti and S. Cannistraro	261 (2000) 39
tallel form	
Nonlinear responses (incl. optical)	
Solvent effect on static vibrational and electronic contribution of first-order	
hyperpolarizability of π -conjugated push-pull molecules: quantum-chemical calculations. W. Ponthawigh and T. Misiagrah	261 (2000) 252
tions, W. Bartkowiak and T. Misiaszek Calculation of macroscopic linear and nonlinear optical susceptibilities for the	261 (2000) 353
naphthalene, anthracene and meta-nitroaniline crystals, H. Reis, M.G. Papadopou-	
los, P. Calaminici, K. Jug and A.M. Köster	261 (2000) 359
105, 1. Calaminici, R. Jug and A.M. Roster	201 (2000) 339
Multiphoton phenomena	
Formation of long-lived Rydberg states of H ₂ at K impregnated surfaces, J. Wang and	
L. Holmlid	261 (2000) 481
Reactions (incl. dissociation)	
Density functional studies on the mechanisms of unimolecular reactions of HXCSe	
(X = H, F, Cl, and Br), HY. Liao, MD. Su and SY. Chu	261 (2000) 275
Processors for engine language with a granter of a stage and	
-condensed phase	261 (2000) 201
Random walks and reactions on dendrimer structures, P. Argyrakis and R. Kopelman	261 (2000) 391
Tunneling	
Influence of the guest molecule on the rotational potential for NH ₃ groups in Hofmann	
clathrates, P. Vorderwisch, S. Hautecler, G.J. Kearley and F. Kubanek	261 (2000) 157
Structure of trihalogenomesitylenes and tunneling of the methyl groups protons, J.	
Meinnel, M. Mani, A. Cousson, F. Boudjada, W. Paulus and M. Johnson	261 (2000) 165

Electron transfer	
The influence of conformation and energy gaps on optical transition moments in donor-acceptor biphenyls, M. Maus and W. Rettig	261 (2000) 323
Photoinduced formation of persistent contact ion pairs in solid noble gases: UV/Vis	201 (2000) 323
spectroscopic, photokinetic and energetic investigations, B. Gödicke, A. Langenscheidt, H. Meyer and A. Schweig	261 (2000) 339
Ionization (incl. Rydberg states)	
Electron momentum spectroscopy study of amantadine: binding energy spectra and valence orbital electron density distributions, I.V. Litvinyuk, Y. Zheng and C.E. Brion	2(1 (2000) 200
	261 (2000) 289
Mass analyzed threshold ionization spectroscopy of 4-aminobenzonitrile cation, L.C.L.	261 (2000) 440
Huang, J.L. Lin and W.B. Tzeng	261 (2000) 449
Formation of long-lived Rydberg states of H ₂ at K impregnated surfaces, J. Wang and	261 (2000) 401
I. Holmlid	261 (2000) 481
Molecular motion (incl. diffusive)	
Methyl group dynamics above the glass transition temperature: a molecular dynamics	
simulation in polyisoprene, F. Alvarez, A. Arbe and J. Colmenero	261 (2000) 47
A comparison of neutron scattering studies and computer simulations of polymer melts,	
G.D. Smith, W. Paul, M. Monkenbusch and D. Richter	261 (2000) 61
Adsorption of ethane and ethene in Na-Y studied by inelastic neutron scattering and	
computation, N.J. Henson, J. Eckert, P.J. Hay and A. Redondo	261 (2000) 111
Molecular dynamics simulation study of cyclohexane guest molecules in the	()
cyclohexane/thiourea inclusion compound, JC. Soetens, A. Desmedt, F. Guillaume	
and K.D.M. Harris	261 (2000) 125
Diffusion in aqueous solutions of 1,2-dimethoxyethane: comparison of molecular	
dynamics simulations and quasielastic neutron scattering, F. Trouw, D. Bedrov, O.	
Borodin and G.D. Smith	261 (2000) 137
Molecular motions in liquid crystal BBBA (40.4): QENS study, S. Mitra, R.	201 (2000) 101
Mukhopadhyay and K. Venu	261 (2000) 149
Graphite intercalation by nitric acid: conduction ESR and theoretical studies, A.M.	201 (2000) 117
Ziatdinov and P.G. Skrylnik	261 (2000) 439
Surface chemical physics	
-surface scattering	
Graphite intercalation by nitric acid: conduction ESR and theoretical studies, A.M.	
Ziatdinov and P.G. Skrylnik	261 (2000) 439
Standard of called limits and almost	
Structure of solids, liquids and glasses Recent developments of the parameters of t	
Recent developments of the RMCPOW method for structural modelling, A. Mellergård	261 (2000) 265
and R.L. McGreevy	261 (2000) 267
Critical behaviour and phase transitions	
Graphite intercalation by nitric acid: conduction ESR and theoretical studies, A.M.	
Ziatdinov and P.G. Skrylnik	261 (2000) 439
	() 10)

Molecular self-assembly and -organization

A modified Poisson-Boltzmann equation. I. Basic relations, S. Woelki and H.-H. Kohler

261 (2000) 411

A modified Poisson-Boltzmann equation. II. Models and solutions, S. Woelki and H.-H. Kohler

261 (2000) 421